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MODELLING THE ALTERATION HALO OF A DIORITE INTRUSION

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SUMMARY

In this paper we first calculate the chemical and physical conditions in a geothermal reservoir containing CO_2. Then we consider the effect of a pulse of magmatic vapour into the base of this reservoir and calculate the changed chemical and physical conditions as the reservoir is allowed to evolve for a further 8,000 years. The chemistry in the reservoir is described by eleven component species, H_2O, H^+, Cl^-, $SO_4^=$, HCO_3^-, HS^-, SiO_2, Al^{+++}, Ca^{++}, K^+ and Na^+. Associated with these components are 32 secondary species and nine minerals.

1. INTRODUCTION

For many years it has been possible to compute the transport of heat and mass within the earth using simulators such as TOUGH2 and TETRAD. Reaction-path simulators are also well advanced, and used as a matter of course by geochemists to unravel the intricacies of the chemistry of fluids within the earth (e.g. Reed 1982, Parkhurst 1995). Recently there has been a growing interest in combining these disciplines to allow the modelling of reactive chemical transport in porous media (e.g. Lichtner (1992), Steefel and Lasaga (1995) Friedly (1989), Friedly and Rubin (1992), White (1995) and Lichner and Seth (1996)

In this paper, we have applied the reactive transport simulator CHEM-TOUGH2 to a problem that is highly relevant to evolutionary development of Taupo Volcanic Zone (TVZ) geothermal systems, that of simulating fluid flow adjacent to a shallowly-seated, degassing magmatic intrusion. Model parameters for this work have been derived in part from the paleo-magmatic heat-source environment in the Ngatamariki system (Christenson et al., 1997; 1998).

2. MODEL DESCRIPTION

Drilling at Natamariki intersected a 700 ka old diorite intrusion at about 2 kilometres below the ground surface. In this work, we model the hydrothermal and chemical system extant above this intrusion soon after emplacement.

We have adopted a cylindrical symmetry for the model. The cylinder has a radius of two kilometres, and extends from the surface to two kilometres depth (Figure 1).

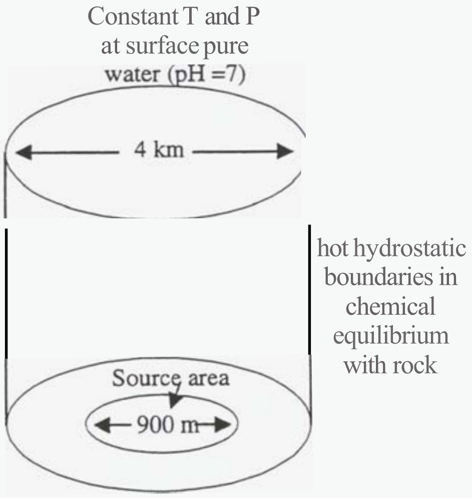

Figure 1: Layout and boundary conditions for Tough2 model.

At the surface we assume water containing no dissolved solids or gases, a pH of 7, a constant temperature of 20°C and a pressure of one bar. On the vertical boundary of the model we assume hydrostatic pressures and temperatures consistent with a temperature gradient of 40°C/km. Fluid on the boundaries is in equilibrium with the rocks which are assumed to make up the unaltered reservoir. No fluid or heat flow is possible across the base of the model except over a central circular region of radius 450 metres at the base where various chemical components enter the modelled region from the degassing intrusion.

The modelled region is divided into ten layers each with a thickness of 200 metres. Each layer is divided into 20 'ring' elements. These elements are smallest near the center of the model and larger towards the boundaries. The upper 200 metres of the reservoir forms a partial cap and has a permeability of 0.01 milli-Darcy. The rest of the reservoir has a permeability of 1.0 milli-Darcy and porosity throughout is 0.1.

Modelling the transport of reactive chemicals is a computer intensive activity, and requires that a balance be struck between chemical complexity and calculation time. For this initial model, we adopted a simplified subset of reservoir component species, including H_2O, H^+, Cl^-, $SO_4^=$, HCO_3^-, HS^-, SiO_2, Al^{+++}, Ca^{++}, K^+ and Na^+. These fluid components allow the modelling of reactions between the main magmatic volatiles (CO_2, SO_2, H_2S, HCl) and the most common rock-forming minerals (albite, anorthite, K-feldspar and **quartz).** Thirty two of the most prevalent secondary aqueous species and 11 alteration minerals are also considered (Table 3).

Simplifying assumptions adopted in the treatment are:

- chemical equilibrium is maintained;
- gas phase chemistry is ignored;
- the reacting minerals exert no direct redox control on the system; and
- reservoir permeability is isotropic (fracture flow is ignored).

Each of these assumptions, of course, represents a significant departure from natural magmatic-hydrothermal systems. In terms of modelling the physical characteristics of the reservoir, perhaps the most important assumption is the exclusion of gas chemistry (boiling may still take place but the effect of dissolved gases, e.g. CO_2 , on boiling point is ignored). However, since the main hydrolysis-promoting agents in the magmatic environment (ie. HCl and SO_2) partition strongly into the liquid phase (Christenson and Wood, 1993), exclusion of boiling from the model does not adversely affect the outcome of the chemical model in the vicinity of the heat source. Obviously this cannot be the case where, at some distance from the heat source, CO_2 becomes the dominant hydrolysis-promoting agent. *As* modelled, the alteration intensities in the distal portions of the model system should be considered as maximum values.

Whereas we believe the assumption of chemical equilibrium to be justified in the hot area of the reservoir, this assumption is certainly invalid in the cool areas. For example, the pH in the cool surface waters is much higher than normally found, but is correct for water in equilibrium with the assumed rock assemblage at 20°C. This, and the other simplifications herein, will be addressed in future refinements of the model.

3. CHEMICAL ENVIRONMENT

The hydrothermal environment within or immediately adjacent to shallow (< **4km)** cooling diorite plutons is characterised by high temperatures **(up** to 1100°C), pressures ranging from hydrostatic to lithostatic (ca. 200 – 2000 bar), and by the presence of highly reactive fluids. In this paper, we consider only the interaction between the volatile species released from a cooling magma, and the overlying hydrothermal environments.

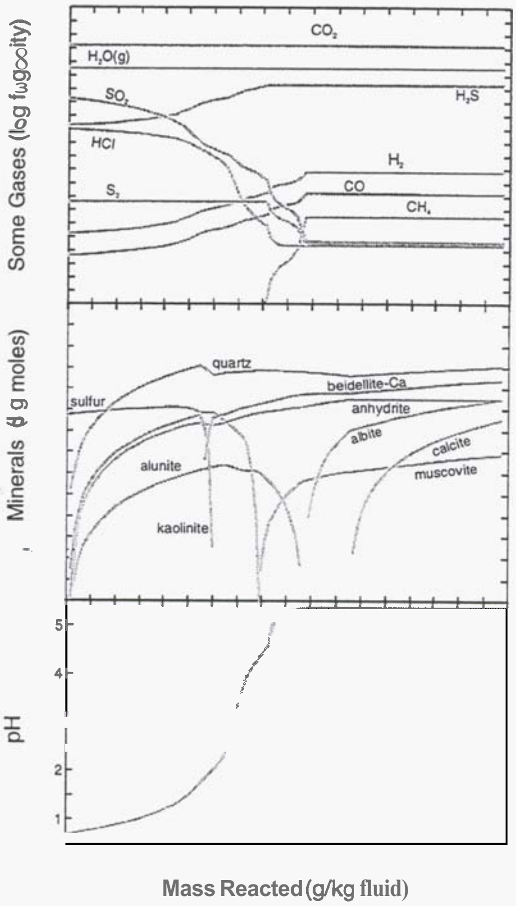

Figure 2. Reaction pathway resulting from titration of 900 g of the simplified mineral assemblage into 1 kg of White Island fumarolic condensate. Calculated at 300 "C. (Giggenbach and Sheppard, 1989).

This is in keeping with evidence from Ngatamariki suggesting that release of magmatic volatiles occurred periodically during the cooling history of the diorite intrusion found there.

Fluid-rock reaction pathways which are typical of these environments are summarised in Figure **2.** Using the reaction path simulation programme REACT (Bethke, 1992), we have numerically titrated 900g of our simplified mineral assemblage (Table **2)** into 1 kg of condensed fumarolic discharge from White Island (fumarole #**3**, Giggenbach and Sheppard, 1989).

The condensate becomes progressively acid-neutralised through the hydrolysis reactions which ensue, during which time an early mineral assemblage consisting of cation-stripped silicates, sulfate minerals and S gives way to an alteration assemblage more typical of present-day TVZ systems (eg. Browne, 1998). The composition of the dissolved gases also changes, reflecting both increasing pH and decreasing redox state of the fluid with reaction progress.

Extending this chemical approach to a reservoir-wide model, whilst maintaining a real sense of time and space (ie. relevance to TVZ systems) required that the **CHEM-TOUGH2** model be done in a series of steps. Firstly, the initial pressure and temperature state of the reservoir was calculated using only the TOUGH2 simulator (Pruess, 1987). Starting with a reservoir at 20°C and hydrostatic pressures the model was run with the source terms specified in Table 1 for the scenario labeled 'initial' until a steady state was reached.

This calculation provided starting temperature and pressure conditions for the second calculation. The aim was to estimate chemical conditions **and** rock alteration products in a single-phase liquid reservoir containing CO_2. The reservoir **rock was** assumed to consist initially of the assemblage given in Table **2.** Heat and mass flows into the reservoir are again given in Table 1 in the row labeled 'CO_2 only'. The flows specified there are equivalent to source fluid containing *3.6%* CO_2 by weight. This model was run to simulate the evolution of the reservoir for 100,000 years, and resulted in the chemical conditions and rock alteration products shown in Figure **3.** The temperatures, pressures aqueous chemical components and mineral assemblage at the end of this simulation provided the initial state of the reservoir prior to intrusion of the diorite.

Name	Composition	Weight %
Albite	$NaAlSi_3O_8$	40
Anorthite	$CaAl_2Si_2O_8$	40
K-feldspar	$KAlSi_3O_8$	*6*
Quartz	SiO_2	14

Table2: Initial rock composition.

4. MAGMATIC INTRUSION

The fluxes of magmatic inputs into the convecting reservoir overlying the intrusion have been normalised to a inter-eruptive SO_2 flux of ***350*** t/d from White Island, as given in Table 1 in the row labeled 'full model'. These gases, with an enthalpy of steam at 350°C, are injected into the model over the source area **for** a period of three years. After this the rate is dropped to 1% of the initial rate and the simulation run for another 8,000 years.

5. RESULTS

Results of the modeling are summarised in Figure **4.** pH and Cl^- contours depict the shape of the convective upwelling over the intrusion. **As** described above, hydrogen ions within the plume are consumed in hydrolysis reactions, and after 8000 years, the distribution of Cl^- in the system shows that the cell has accomplished about one complete convective cycle. The field of K-feldspar dissolution has expanded well beyond that found in the initial state, having been largely replaced by muscovite, which in turn is replaced by kaolinite along the front of advancing acidic fluids. **As** expected, alunite is stable close to the heat source.

Ca^{++} released from the increased dissolution of anorthite is taken up in anhydrite in the low pH zone close to the heat source, and calcite further away. Fluids close to the source are most acidic, with concentration and the distribution of some of the alteration products throughout the reservoir.

Name	Composition
Alunite	$K Al_3(SO)_4(OH)_6$
Anhydrite	$CaSO_4$
Calcite	$CaCO_3$
Kaolinite	$Al_2Si_2O_5$(OH),
Muscovite	$KAl_2(AlSi_3O_{10})(OH)_2$
Pyrophyllite	$Al_2Si_4O_{10}(OH)_2$
Sulfur	S

Table **3:** Rock alteration products included in the calculations.

6. DISCUSSION

We have demonstrated that it is possible, with the assumptions given earlier, to model the chemical changes that take place in a geothermal reservoir in response to a large pulse of magmatic vapour. The chemical modeling includes sufficient detail to represent the processes associated with the neutralisation of the low pH fluids that result from the dissolution of magmatic vapour into reservoir fluid.

The reactive transport approach described herein has implications for future geothermal exploration and development. Not only does it provide us with a predictive capability for "fitting" observed fluid chemistry and alteration products in shallow reservoir environments to unexplored heat source environments at depth, but ultimately it will allow for testing production scenarios in near heat-source environments.

Much more work is required to make the model more realistic but software development is largely complete. CHEM-TOUGH2 is capable **of** modelling the gas-liquid reactions omitted from this work (White and Kissling 1996) and also kinetic reactions (Xu *et al.* 1998). The effect of fluid flow primarily in fractures with diffusion of chemical species into the rock matrix can be handeled using the MINC formalism (Pruess 1983). These issues will be addressed in the near future.

7. ACKNOWLEDGEMENTS

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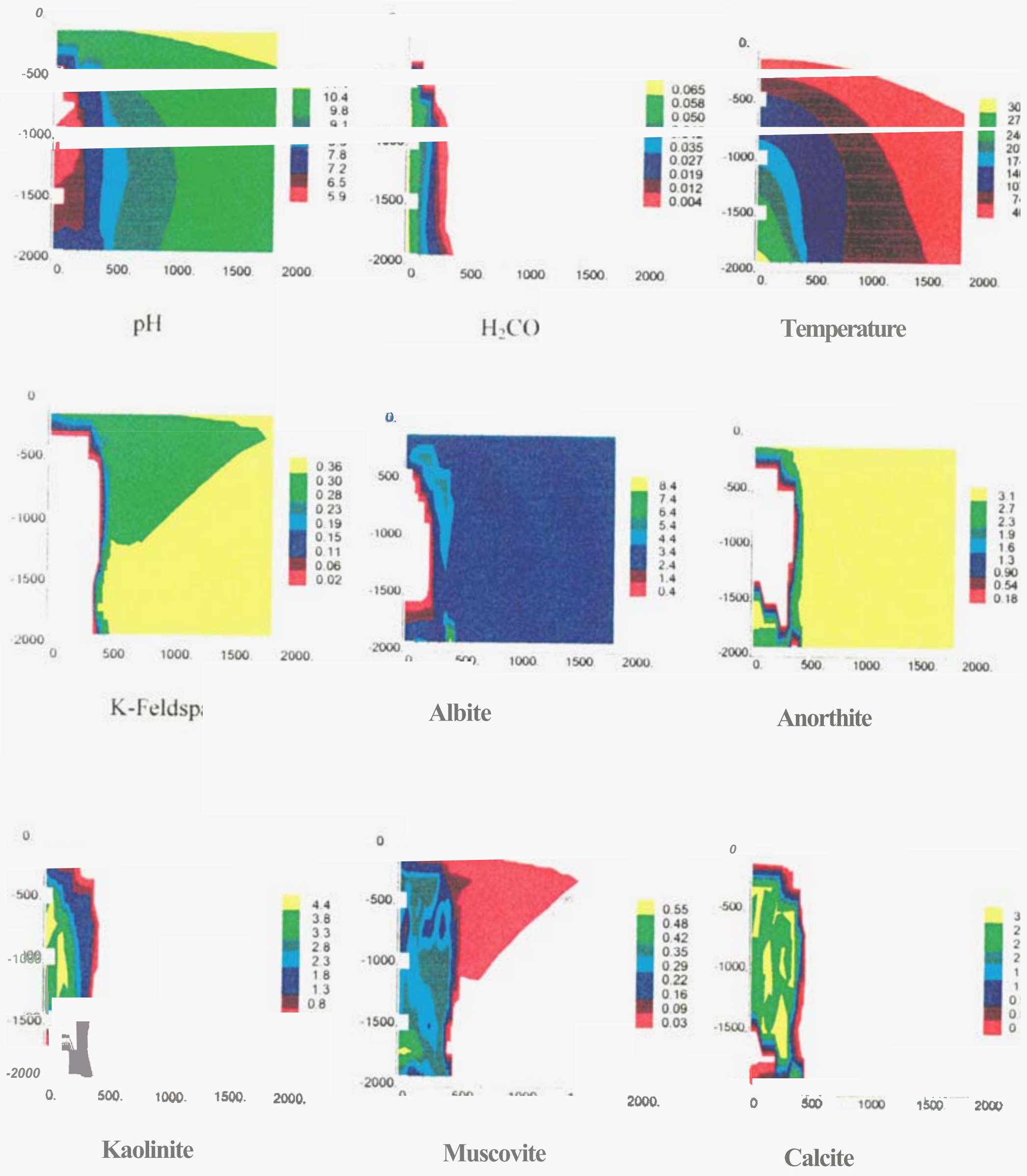
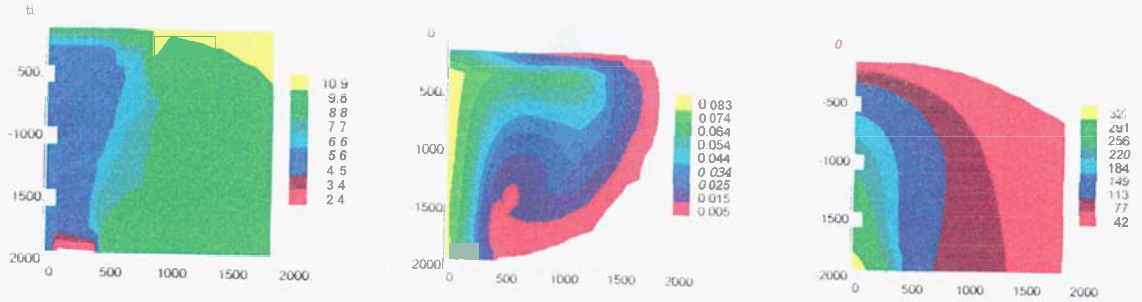


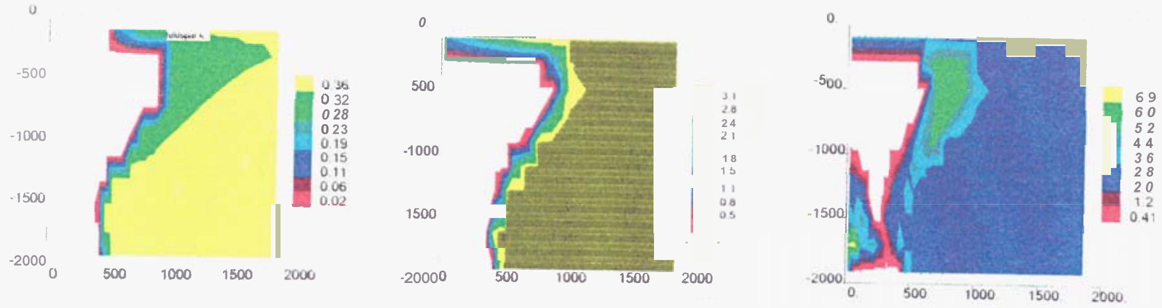
Figure3: **Initial mineral assemblege and some aqueous species concentrations. Aqueous concentrations are in Moles/kg and solid concentrations in Moles/liter of fluid.**

Scenario	Heat (W/m2)	H_2O (kg/sec)	H^+ (kg/sec)	HCO_3^- (kg/sec)	HS^- (kg/sec)	$SO4^=$ (kg/sec)	Cl^- (kg/sec)
Initial	2.0	0.54	0.0	0.0	0.0	0.0	0.0
CO_2 only	2.0	0.54	3.17e-4	1.94e-2	0.0	0.0	0.0
Full model	2.0	152.5	1.33	59.79	2.77	12.87	2.47

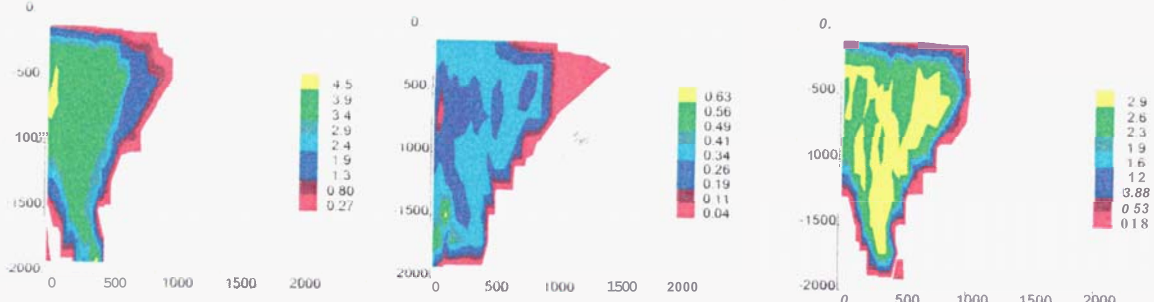
?able 1: Heat and mass flows for the three modelled scenarios.



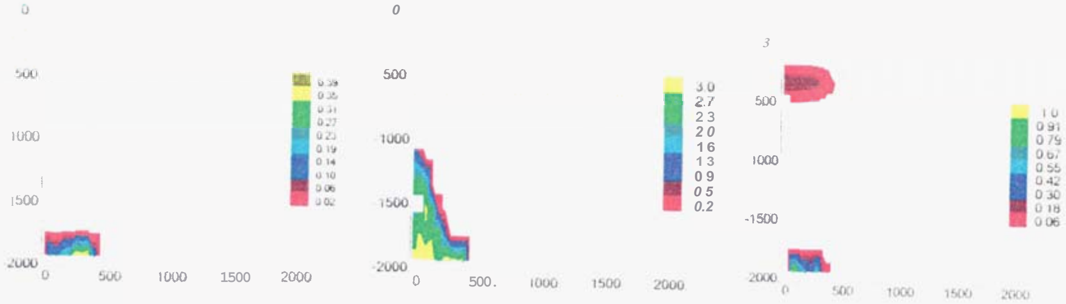
pH Cl- Temperature



K-Feldspar Anorthite Albite



Kaolinite Muscovite Calcite



Alunite Anhydrite Sulphur

Figure 4: Final state of the reservoir 8000 years after pulse of magmatic vapour. Aqueous concentrations are in Moles/kg and solid concentrations in Moles/liter of fluid all distances are given in metres.